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Original Research

Unveiling the Bacterial Communities and Its Potential Agricultural Applications from Organic Manure (Panchagavya) Using Targeted Amplicon Analysis

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Abstract

Due to the alarming effect of synthetic and chemical-based agriculture on human health and the environment, organic farming has been receiving increasing attention around the world. Panchagavya (PG) and farmyard manure play crucial roles in organic farming's nutrient management. Despite its known potential in crop applications, Panchagavya microbial profile has yet to be mapped. The aim of this study is to unveil the succession of bacterial communities in Panchagavya during the fermentation process using targeted amplicon analysis. The results revealed that 45 phyla, 92 classes, 168 orders, 333 families, 899 genera, and 2026 species were obtained from all samples, along with 5144 OTUs. *Proteobacteria* (36.61-70.98%) *and Bacteroidetes* (14.59-23.81%) were found in greater abundance in all samples, with *Proteobacteria* being the most common in all samples, followed by *Bacteroidetes* and *Firmicutes* (12.67-29.58%). *Pseudomonas* was a dominant member of the fermentation process, along with *Romboutsia, Paeniclostridium, Clostridium, Enterococcus, Lactobacillus, Bifidobacterium,* and *Ruminococcus*. The findings indicate that Panchagavya demonstrates effectiveness as a fertilizer due to its inclusion of advantageous microorganisms and growth stimulants for plants. Furthermore, some bacterial members that have not yet been characterized for any role in the soil and plant systems, urging a comprehensive investigation into the potential functions for future agricultural applications and practices.

Keywords: Panchagavya, liquid manure, metagenomics, bacterial communities, organic farming

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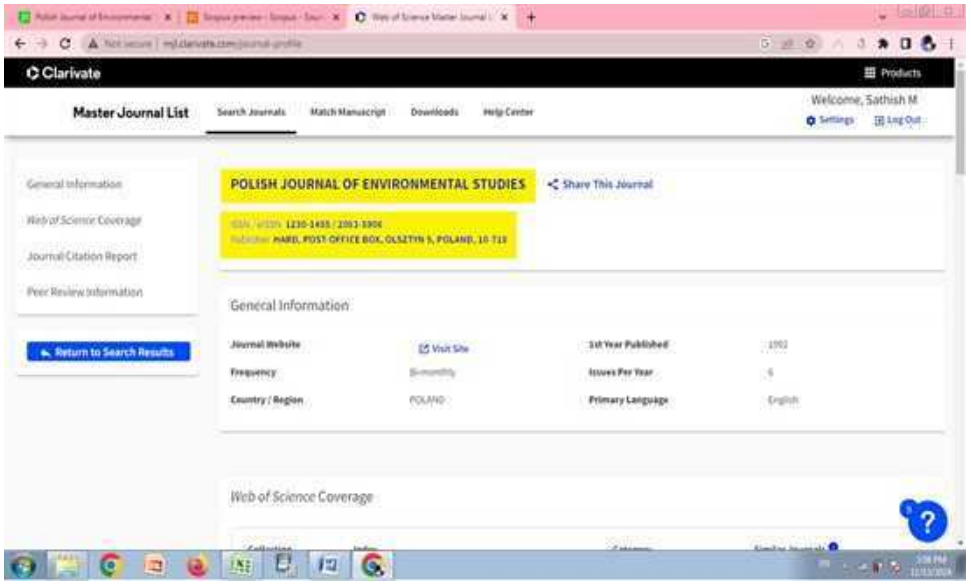

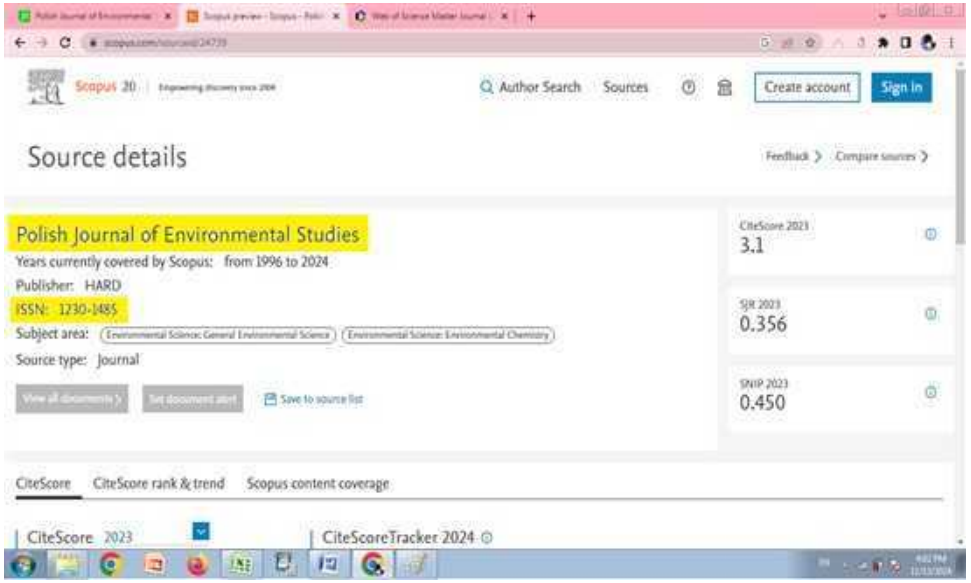

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Brief Report

Unveiling the Potency and Harnessing the Antibacterial Activities of Plant Oils against Foodborne Pathogens

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Abstract: The rising concerns regarding antibiotic resistance and the harmful effects of synthetic preservatives have led to an increasing interest in exploring natural alternatives. Plant oils have been traditionally used for their antimicrobial properties, but systematic investigations into their efficacy against foodborne pathogens are necessary for potential applications in food preservation. This study aimed to evaluate the antibacterial potential of various plant oils (neem, coconut, castor, and olive oil) against common foodborne pathogens and analyze their chemical composition using gas chromatography–mass spectrometry (GC-MS). The oils were tested against foodborne pathogens using the disk diffusion method. Minimum inhibitory concentrations (MICs) were determined to assess the potency of the oils. GC-MS was employed to identify the compounds present in each oil. Neem oil exhibited significant antibacterial activity against all tested pathogens, with pronounced effects against *Staphylococcus aureus* and *Bacillus cereus*. Coconut oil showed notable activity against *Listeria monocytogenes*. Castor oil displayed moderate activity, while olive oil exhibited minimal antibacterial effects. The GC-MS analysis revealed a diverse array of compounds in neem oil, which is likely to contribute to its potent antibacterial properties. Neem and coconut oils, owing to their rich bioactive components, emerged as promising candidates for the development of natural antimicrobial agents. These brief findings support the potential application of plant oils in food preservation and emphasize the need for further research into understanding the underlying mechanisms and optimizing their use.

Keywords: essential plant oils; antibacterial activity; gas chromatography–mass spectrometry (GC-MS); foodborne pathogens; minimum inhibitory concentrations (MICs)

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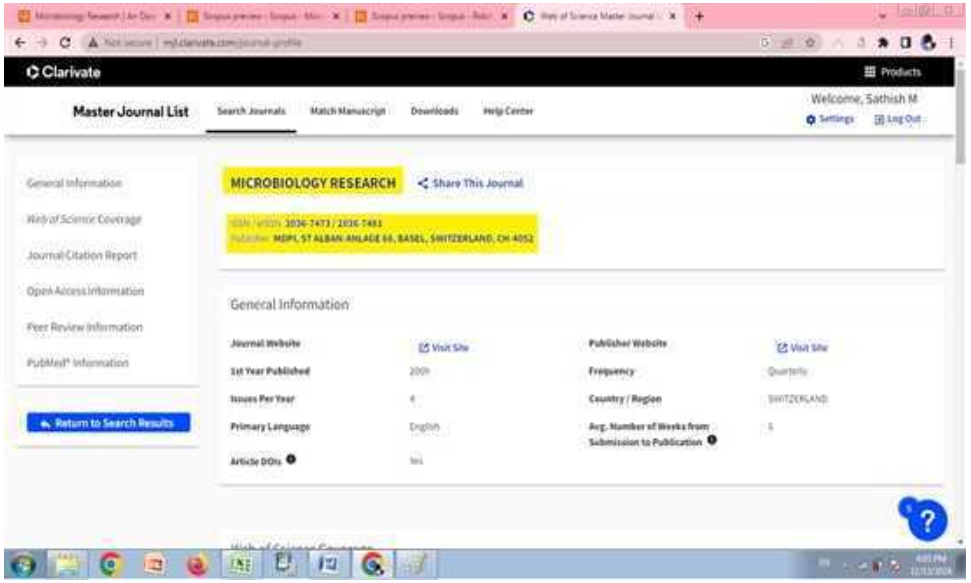
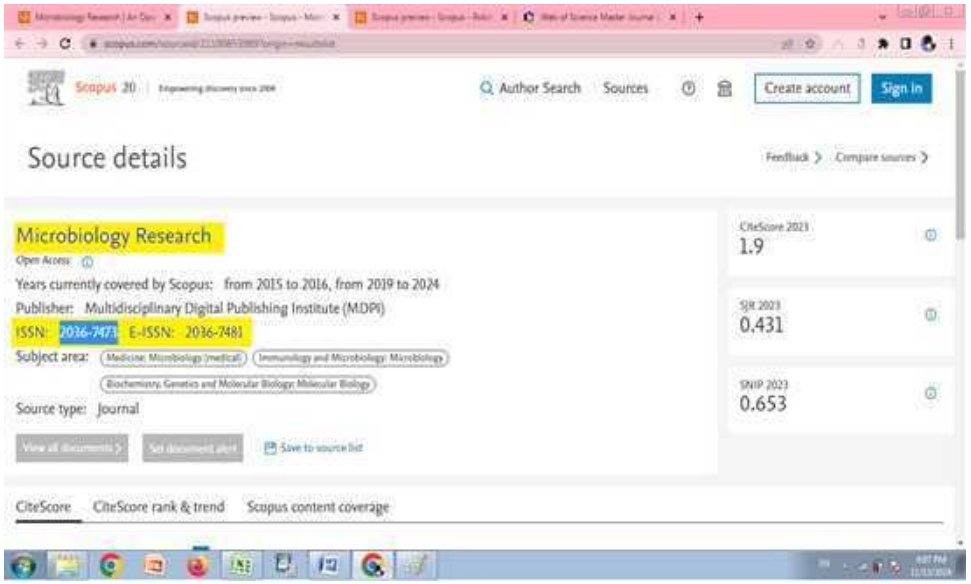
1. Introduction

The impact of microorganisms on food spoilage has captured the attention of food producers and those concerned with sustainable food consumption [1,2]. Throughout history, foodborne diseases have plagued humanity, affecting millions annually through a diverse range of pathogens and physical and chemical agents [3]. The visual symptoms exhibited by spoiled food provide clear evidence of the spoilage process. Biochemical reactions, such as oxidation, which commonly occur during food processing and storage, contribute to reducing product shelf life and the deterioration of flavor, texture, and color [4]. The proliferation of pathogenic bacteria and fungi in food threatens its preservation and contributes to the emergence of foodborne diseases worldwide [1]. Increasing consumer apprehension regarding the side effects of chemical and synthetic preservatives has fueled the demand for natural alternatives [5]. Thus, there is an urgent need to identify natural substances





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Isolation and characterization of rhizosphere soil associated phosphofungi from hybrid brinjal *Solanum melongena* L. var. MDU1

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The current study focuses on isolation and identification of potent filamentous fungi from the rhizosphere soils associated with high yielding hybrid brinjal (*Solanum melongena* var. MDU1) plants to solubilize tricalcium phosphate (TCP) under *in vitro* conditions using Pikovskaya (PVK) medium. A total of 68 fungal isolates were obtained from 15 rhizosphere soil samples from three *S. melongena* fields, and they demonstrated a clear halo zone of dissolved phosphate solubilization in PVK medium, indicating that these fungi had the requisite P-solubilizing ability. Among, maximum solubilization index (SI%) of TCP on PVK plates was recorded with the fungal isolate *Aspergillus* spp. (TSPS 2) with 2.3%, whereas the lowest of 0.9% was detected from the isolate *Trichoderma* spp. (TSPS 9). In addition, quantitative TCP solubilization in PVK broth inoculated with *Aspergillus* spp. (TSPS 2) revealed higher amount of P mobilization ranged between (216.43–490.56 µg/mL^{-1}) in different days of incubation. Similarly, found the greatest decline in pH from an initial pH of 7.0 to 4.5 at varied time interval. The current investigation found a variety of plant-soil-associated P-solubilizing fungi that could be used as biofertilizers.

Keywords: *Aspergillus* spp., crop plants, phosphate solubilization, rhizosphere soil

INTRODUCTION

Phosphorus (P) is naturally occurring and one of the most indispensable macronutrients next to nitrogen among 17 elements that are essential for the growth and development of plants. It is one of the major limiting factors for crop production on many tropical and subtropical soils (Yasser *et al.* 2014).

It accounts for 0.2% of plant dry weight and restricts plant growth and agricultural productivity (Pradhan and Sukla, 2006). A greater part of soil phosphorus, approximately 95–99%, is present in an insoluble form complexed with cations like iron (Fe), aluminum (Al), and calcium (Ca) that cannot be utilized by plants (Gizaw *et al.* 2017). Plant mineral nutrition is mostly determined by soil P content, which can be digested as soluble phosphate (Wang *et al.* 2018). Furthermore, P contributes significantly to photosynthesis, energy and sugar production, nucleic acid synthesis, N2 fixation in legumes, and plant disease resistance (Kanse *et al.* 2015).

Phosphorus is the kingpin of Indian agriculture, with a unique role in both traditional and alternative agriculture (Pradhan and Sukla, 2006). A large variety of microbial species have been identified in soil, particularly in the rhizosphere, where soil plays an important role in P solubilization (Yasser *et al.* 2014). Phosphate solubilizing microorganisms (PSM) use a unique process to transform these insoluble phosphates into soluble forms. That is, they carry out the acidification, chelation, exchange reaction, and gluconic acid synthesis processes (Elias *et al.* 2016; Sabbir *et al.* 2022). The organic acids and inorganic acids produced by bacteria convert tri-calcium phosphates into di- and monobasic phosphates, resulting in increased

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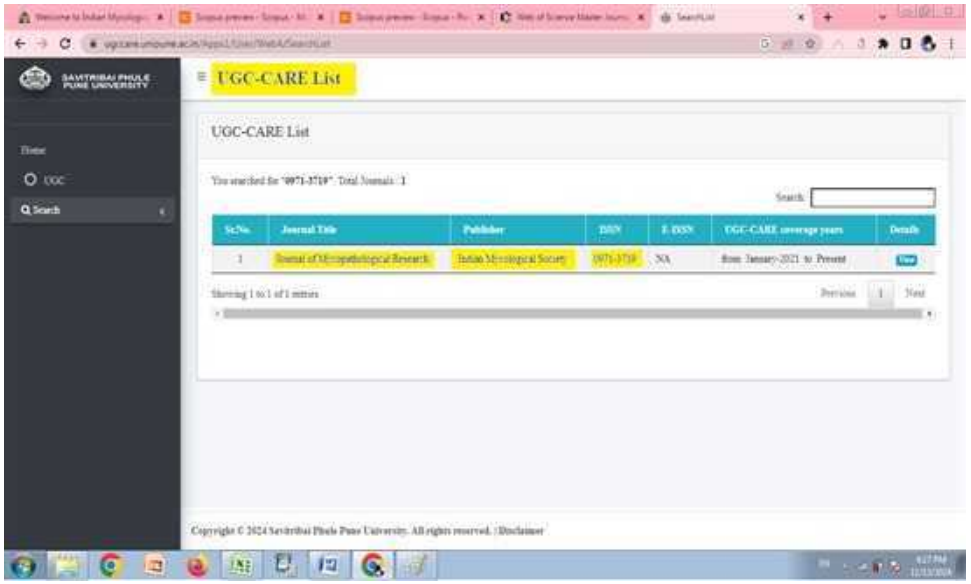

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Assessment of root colonization, identification, and phosphate solubilization activity of root endophytic fungi obtained from hybrid tomato *Lycopersicon esculentum* Mill. var. TNAU CO3

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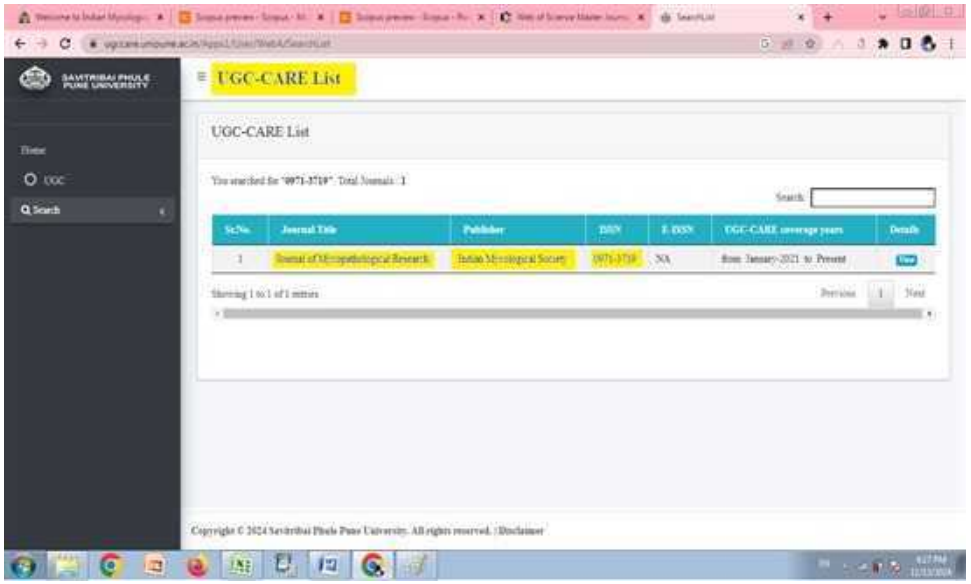
Land plants, in general, rely heavily on positive interactions with fungal endophytes for growth, disease resistance, and stress tolerance. Root colonization, isolation and tri-calcium phosphate (TCP) solubilizing activity of root endophytic fungi (REF) obtained from hybrid tomato (*Lycopersicon esculentum* Mill. var. TNAU CO3) plants grown in natural fields were examined. All field-collected tomato roots were positively colonized by DSE (dark septate endophyte) fungi. A total of 94 culturable fungal isolates belonging to 8 distinct orders, 9 genera, and 11 species were recovered and identified by morphological examination. In *L. esculentum* roots, the endophytic fungal colonization rate (CR%) was noticeably high (62.67%). *Aspergillus niger* was the dominant fungus with a relative abundance (RA%) of 23.4%, while *A. niger*, *Cladosporium cladosporioides*, and *Fusarium oxysporum* had the maximum isolation frequency (IF%). Furthermore, we evaluated the nature of the identified fungal isolates as endophytes by a pot study. Thus, 9 of 11 fungi colonized the test plant roots with clear intracellular structures, including *Alternaria* spp., *C. cladosporioides*, *Colletotrichum* spp., and *F. oxysporum*, which are DSE fungi. Furthermore, four REF were able to solubilize the TCP, with SI% ranging from 1.3 to 2.4%. This study's findings will help to improve our understanding of REF interactions and their potential ability to solubilize inorganic phosphate, as well as the application of these fungi to increase the development and productivity of diverse agricultural plants in sustainable agriculture.

Keywords: Dark septate endophyte fungi, crop plants, colonization, PVK agar, phosphate soubilization



INTRODUCTION

Plant roots are quickly colonized in natural habitats by a vast range of microorganisms, including archaea, bacteria, and endophytic fungus, known as the plant microbiome (Liu *et al.* 2017). Arbuscular mycorrhizal (AM) fungi, the most widespread endophytic fungi in plant roots, form symbioses with about 90% of plant species in all habitats (Smith and Read, 2008).

However, dark septate endophytes (DSE) or root-endophytic fungi (REF) also colonize plant roots alongside AM fungi in tropical, arctic, and alpine habitats (Addy *et al.* 2005; Newsham, 2011). Darkly colored (melanin), septate hyphae, and compact microsclerotial structures define DSE fungi. Plants grown in extreme environments, like heavy metal-polluted soils, low nutrient and high salinity soils, upland agroecosystems, and cold conditions, etc., have high DSE prevalence in their roots. It has also been hypothesized that DSE are mostly non-mycorrhizal plant root-inhabiting fungus.

The majority of previous studies on endophytic fungi have focused on their isolation from aerial plant parts (leaf, stem, flower) and from various crop species such as chilli (*Capsicum annuum*) (Paul *et al.* 2012), potato (*Solanum tuberosum*) (Yasser *et al.* 2019), rice (*Oryza sativa*, *Oryza granulate*) (Naik *et al.* 2009; Yuan *et al.* 2010),

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RESEARCH ARTICLE

Comparative study of organic manure (cow dung, goat dung and chicken manuare) on the vegetative growth of *Amaranthus dubius* L

Ramadevi S[1*], Sivaranjani S[2], Vijaya Samoondeeswari S[3], Ramabhai V[4], Arulnangai R[5], Murugesan R[5]

Ramadevi S, Sivaranjani S, Vijaya Samoondeeswari S, et al. Comparative study of organic manure (cow dung, goat dung and chicken manuare) on the vegetative growth of *Amaranthus dubius* L. AGBR.2023;39(4):1-7.

The study's overarching goal is to examine the effects of three different types of organic fertilizer on the growth of *Amaranthus dubius* vegetative parts. On a split plot, we applied five different amendments: None (M_1), cow dung (M_2), chicken dung (M_3), goat dung (M_4), and an equal quantity of cow dung, chicken dung, and goat dung (M_5), all at 2 kg N/ha. Experiments showed that Nitrogen (N), Potash (K_2O), Organic Carbon (C), and Phosphorus (P), as well as stem and leaf length and breadth and number of leaves, were all substantially ($P<0.01$) enhanced after applications of these organic manures. The measurements taken included the height of the plant (10.1 cm to 43.2 cm), the breadth of the stem (2.1 cm to 5.9 cm), and the length of the leaves (6.2 cm to 12.1 cm), the width of the leaves (2.7 to 8.9 cm), and the number of leaves per plant (5 to 12). Plants grown with goat manure (M_4) were shown to have greater mean values for N, K_2O, C, and P, stem length, stem width, leaf length, leaf width, and the number of leaves per plant compared to values obtained from treatments with other organic manures. Across the board, goat dung outperformed dairy cow manure and chicken manure in the evaluations. This factored into the variation in the amendments' total nitrogen, potassium, phosphorus, and carbon content. The greatest responses in the field experiments occurred after the third crop harvest, which is consistent with an increase in organic N and P mineralization over time.

Keywords: Agriculture, *Amaranthus dubius*, Fertilizer, Nitrogen, Potassium, Phosphorus

INTRODUCTION

Amaranthus has 70 species in 3 subgenera. Self-pollinated, it has male and female blooms. Raw or slightly cooked leaves and stems are nutritious. Animals and humans eat *Amaranthus*. Calcium, iron, phosphorus, and carotenoids are abundant. Lysine and sulfur containing amino acids are abundant in *Amaranthus* grains. Fat rich *Amaranthus* contains 6%-10% oil and 77% polyunsaturated fatty acid. Linoleic acid is necessary. Deficits in this lipid cause several health problems. Future crops include *Amaranthus*. *Amaranthus* grain and leaves are global orphan crops. Farmers like *Amaranthus* for its qualities, growth rate, and C4 photosynthesis, usage of grain and leaves, and environmental stress tolerance. Seeds contain beneficial chemicals that reduce chronic illness risk. Short branches and scattered branches distinguish *Amaranthus dubius*. It grows quickly and produces many seeds. Seedlings sprout 2-3 days after seeding. It was edible after 10-15 days. In Tamil Nadu, stems and leaves are boiled for 4-5 minutes and eaten with rice. It was beneficial for farmers, particularly small scale and rural farmers. Because it grows quickly, requires little investment, and is marketable. It's rich in vitamins, notably A. It prevents and preserves eye health. The leaves have 3 times more vitamin C than spinach, 18 times more vitamin A, 20 times more calcium, and 7 times more iron than lettuce. Other *Amaranthus* seeds are larger. It is less drought resistant than a cruentus. Organic manures are cheap and sustainable. They replace expensive inorganic fertilizers. Plants absorb inorganic fertilizers animal waste is a big pollutant. Recycling animal waste improves soil texture, productivity, and the environment. In Asia, organic manure is one of the essential sectors for agricultural conservation and has played a vital part in plant nutrition. Asia is one of the primary nations that generate ~51% of plant accessible nutrients of the world's total rate from industry, notably chicken industries. But the application of inorganic fertilizer continually will lead to loss of soil fertility. Soil productivity depends on soil condition, fertilizer type, organic matter, and plant kind. Organic manure is a zero cost (or) low cost additive. The excrement of plants and animals was left to decompose for weeks to months. High nutrition manure was generated.

Manure contains microbiota from plant and animal waste. It helps farmers maximize productivity and preserve nutritional levels. Because they cannot afford chemical fertilizers, impoverished nations prescribed organic manure. Organic manure is made from agricultural, poultry, food, rice, sugar, and cotton industry wastes. Farmers prefer direct nutrient inorganic fertilizers. Plants quickly absorbed nutrients. However, excessive chemical fertilizer usage caused environmental issues. Some fertilizers include heavy metals and large quantities of radionuclides. Cow dung is excreta of poultry animals, and it is a low cost bio resource. It has a broad variety of microbiota and many of them are advantageous to both humans and crops. Many bacteria can enrich the soil. The cow dung microbiome includes *Enterobacter aerogenes*, *E. coli*, *Citrobacter koseri*, *Klebsiella oxytoca*, *Klebsiella pneumoniae*, *Rhyzobia* spp., *Pasteurella* spp., *Providencia alcalifaciens*, *Pseudomonas* spp., *Providencia stuartii*, *Morganella morganii*, and others [1].

Goat manure is abundant. It's often applied a week before planting. It may maximize plant nutrient uptake after crushed goat dropping pellets. Crop growth rose. Stress resistant and product quality measurable. Goat dung increased sodium, calcium, magnesium, potassium, and phosphorous in soil. Small scale farmers and rural residents benefited. Chicken excrement, rich in N, P, and K, was a key plant nutrition source. Manure has 30%-50% nitrogen and was widely accessible [2]. Micronutrients condition the soil. Chicken droppings are tiny and biodegradable. Unlike cow and goat excrement, it directly feeds plants. It's a potent nutritional source, so utilize it properly. This component maximizes nutrient usage and agro economic status. Due to its high micronutrient content, chicken manure is popular. It boosts soil water soluble salts. High chicken manure will impact seed germination and root development. It's an excellent soil amendment when utilized properly. It increases soil and foliage nutrients, notably N, P, K, Ca, and Mg. Ammonia from chicken dung increases land nitrogen levels. Seed germination will suffer metabolic issues. To reduce the nutritional value, manure must be watered. It will help dilute chicken manure's vitality. Thus, the reaction of red amaranth to manures (cow dung, chicken manure, and oil cake) in the presence of N, P, and K and its influence on soil quality in the old Brahmaputra flood plains, Bangladesh, was studied [3].

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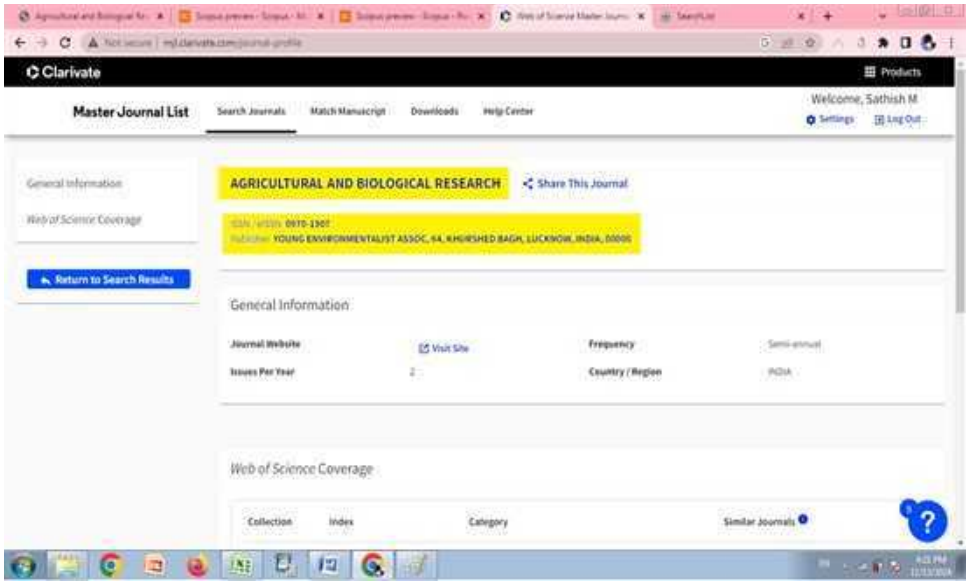

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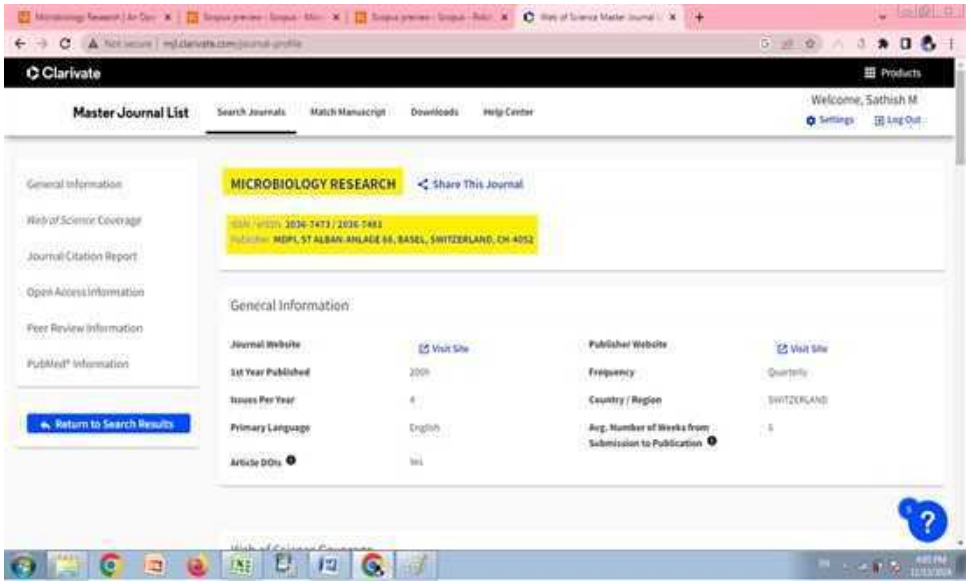

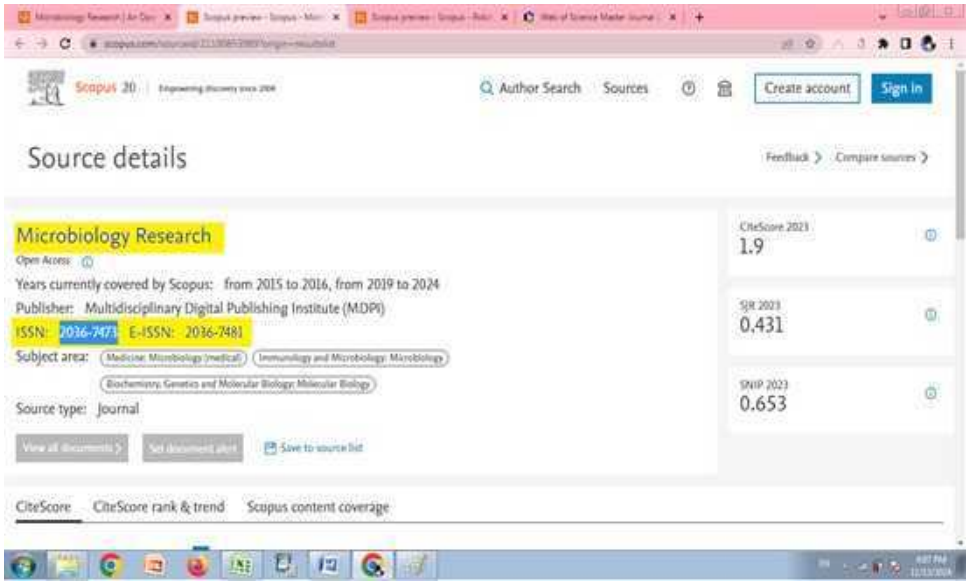

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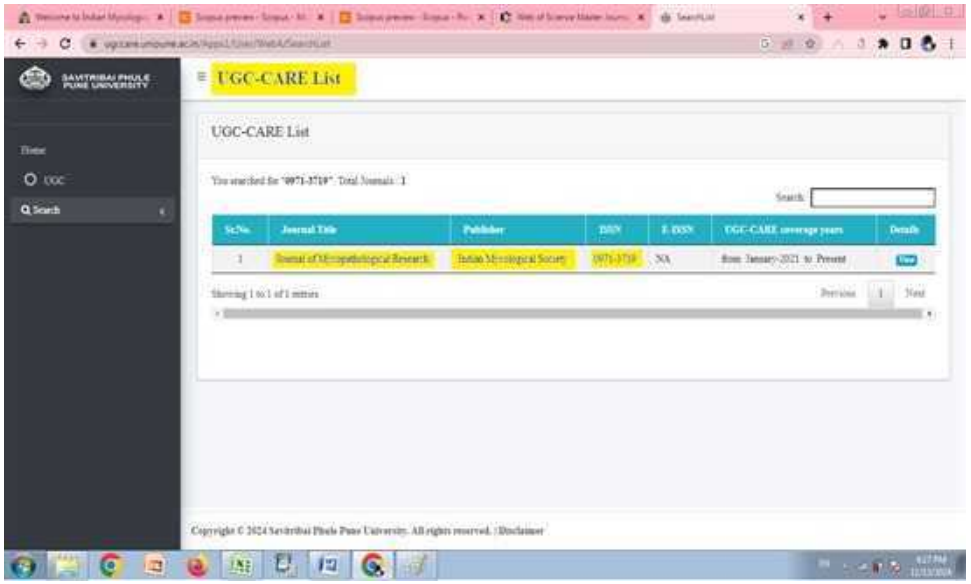
The current study focuses on isolation and identification of potent filamentous fungi from the rhizosphere soils associated with high yielding hybrid brinjal (*Solanum melongena* var. MDU1) plants to solubilize tricalcium phosphate (TCP) under *in vitro* conditions using Pikovskaya (PVK) medium. A total of 68 fungal isolates were obtained from 15 rhizosphere soil samples from three *S. melongena* fields, and they demonstrated a clear halo zone of dissolved phosphate solubilization in PVK medium, indicating that these fungi had the requisite P-solubilizing ability. Among, maximum solubilization index (SI%) of TCP on PVK plates was recorded with the fungal isolate *Aspergillus* spp. (TSPS 2) with 2.3%, whereas the lowest of 0.9% was detected from the isolate *Trichoderma* spp. (TSPS 9). In addition, quantitative TCP solubilization in PVK broth inoculated with *Aspergillus* spp. (TSPS 2) revealed higher amount of P mobilization ranged between (216.43–490.56 µg/mL^{-1}) in different days of incubation. Similarly, found the greatest decline in pH from an initial pH of 7.0 to 4.5 at varied time interval. The current investigation found a variety of plant-soil-associated P-solubilizing fungi that could be used as biofertilizers.

Keywords: *Aspergillus* spp., crop plants, phosphate solubilization, rhizosphere soil



INTRODUCTION

Phosphorus (P) is naturally occurring and one of the most indispensable macronutrients next to nitrogen among 17 elements that are essential for the growth and development of plants. It is one of the major limiting factors for crop production on many tropical and subtropical soils (Yasser *et al.* 2014).

It accounts for 0.2% of plant dry weight and restricts plant growth and agricultural productivity (Pradhan and Sukla, 2006). A greater part of soil phosphorus, approximately 95–99%, is present in an insoluble form complexed with cations like iron (Fe), aluminum (Al), and calcium (Ca) that cannot be utilized by plants (Gizaw *et al.* 2017). Plant mineral nutrition is mostly determined by soil P content, which can be digested as soluble phosphate (Wang *et al.* 2018). Furthermore, P contributes significantly to photosynthesis, energy and sugar production, nucleic acid synthesis, N2 fixation in legumes, and plant disease resistance (Kanse *et al.* 2015).

Phosphorus is the kingpin of Indian agriculture, with a unique role in both traditional and alternative agriculture (Pradhan and Sukla, 2006). A large variety of microbial species have been identified in soil, particularly in the rhizosphere, where soil plays an important role in P solubilization (Yasser *et al.* 2014). Phosphate solubilizing microorganisms (PSM) use a unique process to transform these insoluble phosphates into soluble forms. That is, they carry out the acidification, chelation, exchange reaction, and gluconic acid synthesis processes (Elias *et al.* 2016; Sabbir *et al.* 2022). The organic acids and inorganic acids produced by bacteria convert tri-calcium phosphates into di- and monobasic phosphates, resulting in increased

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RESEARCH ARTICLES

Distribution, molecular characterization and phosphate solubilization activity of culturable endophytic fungi from crop plant roots in North East (NE) India

Kannaiah Surendirakumar[1,2] · Radha Raman Pandey[2] · Thangavelu Muthukumar[3]

Received: 19 January 2023 / Revised: 13 September 2023 / Accepted: 15 September 2023

Abstract
The land plants are highly dependent on beneficial interactions with fungal endophytes for growth, disease resistance, and stress tolerance. We investigated the distribution and tri-calcium phosphate (TCP) solubilizing activity of root-endophytic fungi (REF) isolated from *Capsicum chinense*, *Oryza sativa* cv. Chakhao amubi, *Vigna unguiculata*, and *Zea mays* cultivated in Manipur, North East India. A total of 276 culturable fungal endophytes belonging to eight different orders, 11 families, 17 genera, and 29 species were recovered and identified by morphological and phylogenetic analyses. The isolation rate (IR%) and colonization rate (CR%) of endophytic fungal communities were highest in the roots of *O. sativa* (42% and 68.7%) and lowest in *C. chinense* (12% and 41%). plants, respectively. Likewise, the richness of endophytic fungi was also high in *O. sativa* (21 species) roots. *Fusarium oxysporum* was the dominant fungus with a relative abundance of 22.27%, while *A. niger* recorded the maximum isolation frequency. The diversity indices of identified REF from different crop plant roots were also positively studied. In addition, we microscopically evaluated the percentage of dark septate endophyte (DSE) fungal colonization in crop roots. Further, eight REF were able to solubilize the TCP with solubilization index (SI%) ranging from 1.5 to 2.7%. The findings of this study will contribute to a better understanding of REF interactions and their potential ability to solubilize inorganic phosphate, as well as to the use of these fungi to promote the growth and yield of various crop plants in sustainable agriculture.

Keywords Endophytes · DSE · Diversity · Phylogeny · Solubilization index · Crop species

Introduction

In natural ecosystems, the plant roots are readily colonized by a diverse spectrum of microorganisms, including archaea, bacteria, and endophytic fungi, known as the plant microbiome. The most common type of endophytic fungi in plant roots is the arbuscular mycorrhizal (AM) fungi, which forms symbiosis with more than 90% of the plant species occurring in all the ecosystems (Jumpponen et al. 2017). Fossil and molecular evidence suggest that AM fungal associations were widespread and evolved approximately 460 million years ago, allowing plants to colonize land. The influence of AM fungal symbiosis on a range of plant species (trees, shrubs, and crops), and ecosystems has been well documented (Muthukumar and Tamilselvi 2010). However, growing awareness has revealed that a diverse group of ascomycetous fungi, known as dark septate endophytes (DSE) or root-endophytic fungi (REF), also colonize plant roots alongside with AM fungi growing in a wide range of tropical to arctic, and alpine habitats (Addy et al. 2005; Newsham 2011). The association of DSE fungi can be easily distinguished by their darkly-pigmented (melanin), septate hyphae, and compact microsclerotial structures (Jumpponen et al. 2017). Plants growing in extreme environments, such as heavy metal-polluted soils, low nutrient and high salinity soils, high-altitude forests, upland agroecosystems, cold conditions, etc., have high prevalence of DSE presence in

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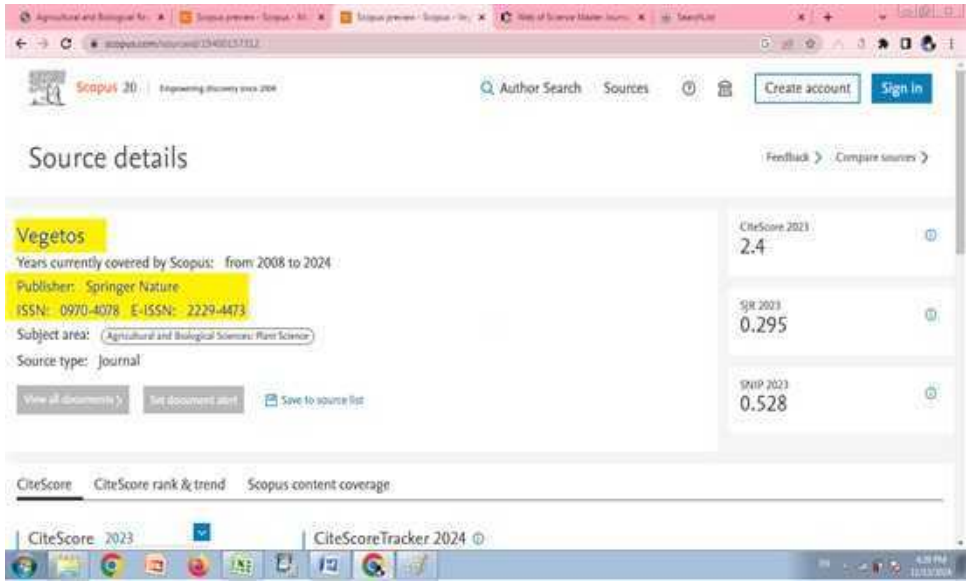

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SYNTHESIS AND CHARACTERIZATION OF DIFFERENT (CU, ZN AND AG) NANOPARTICLES USING *GREWIA CARPINIFOLIA* LEAVES EXTRACT AND THEIR ANTI-MICROBIAL ACTIVITY

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ABSTRACT : The escalating issue of antibiotic resistance has prompted a quest for innovative antimicrobial solutions. Among these, nanoparticles produced through environmentally friendly methods have garnered significant interest for their potential antimicrobial attributes. This investigation centers on the production of distinct nanoparticles ($CuSo_4$, $ZnSo_4$, $AgNo_3$) using the leaves of *Grewia carpinifolia* Juss. The biosynthesized different nanoparticles derived from *Grewia carpinifolia* leaves were subjected to comprehensive characterization through various techniques.

In the UV-visible spectrum analysis, the silver nanoparticles exhibited maximum absorption at 290 nm, copper nanoparticles exhibited their absorbance peak at 310 nm and zinc nanoparticles displayed their peak at 340 nm. XRD analysis indicated that the silver particles generated in our experiments existed in the form of nanocrystals, as evidenced by peaks at 2θ values of 13.8, 21.1, 22.6, 27.2, 29.2, 32.0, 37.8 and 43.6, corresponding to heights of 61.9, 218.0, 172.0, 252.1, 73.9, 604.9, 662.8 and 174.4 counts, respectively. Copper particles exhibited peaks at 2θ values of 9.0, 11.5, 14.2, 15.5, 20.6, 22.6, 27.9 and 29.1, with heights of 44.1, 109.6, 95.9, 103.9, 306.2, 154.7, 132.8 and 199.5 counts, respectively. Zinc particles displayed peaks at 2θ values of 6.9, 9.2, 11.4, 15.4, 18.9, 22.7, 24.9 and 26.5, with heights of 50.2, 440.9, 188.8, 305.4, 440.9, 344.5, 197.6 and 275.5 counts, respectively.

SEM spectral analysis unveiled the formation of cube-shaped silver nanoparticles within a size range spanning from 200 nm to 20 µm. The antimicrobial efficacy of metallic nanoparticles derived from Grewia carpinifolia was evaluated using the disc diffusion method against both gram-positive and gram-negative pathogens, including *E. coli*, *Staphylococcus aureus*, *Bacillus subtilis*, as well as the fungi *Aspergillus flavus* and *Candida albicans*. Notably, metallic Zn, Cu and Ag nanoparticles exhibited substantial zones of inhibition against the selected pathogens, with the highest inhibition zone observed in the case of silver nanoparticles.

Key words : Synthesis, *Grewia carpinifolia*, nanoparticles characterization, antimicrobial activity.

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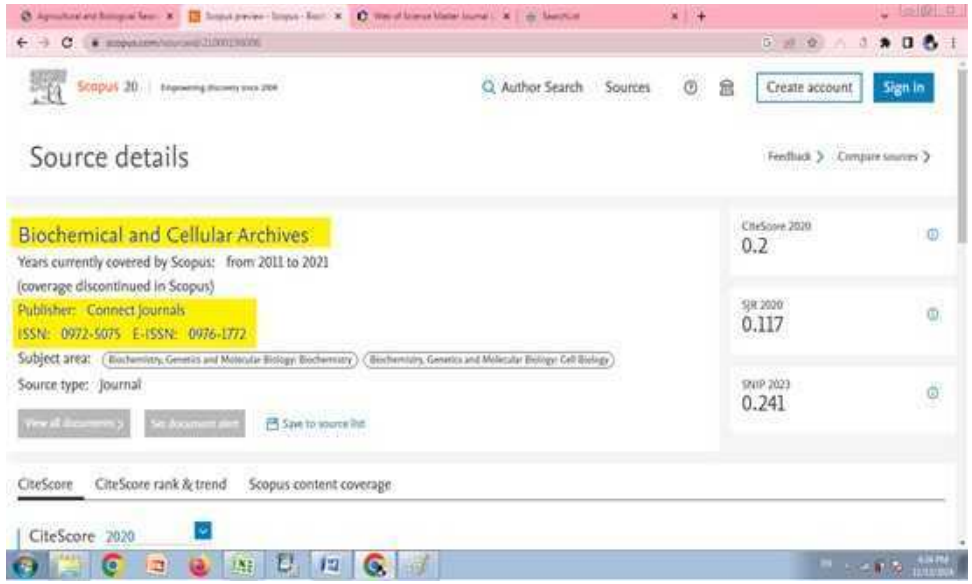

INTRODUCTION

Phyto-mediated synthesis has emerged as a rapid, convenient and widely accepted approach for producing metal nanoparticles. In recent times, various plant components such as bark, leaves, fruits, stems, and seed extracts have demonstrated successful applications in the synthesis of metal nanoparticles (Mittal *et al*, 2013). Among these, silver (Ag) nanoparticles have gained significant attention due to their remarkable antibacterial (Mohanta *et al*, 2016a,b), antifungal and antiproliferative properties (Kim *et al*, 2007; Nayak *et al*, 2015). Leveraging their excellent antimicrobial attributes, silver nanoparticles have found extensive use in food packaging, food and seed preservation, biofertilizers, cosmetics and

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RESEARCH ARTICLES

Exploring the *in silico* studies of the endophyte fungus *Phoma herbarum* against mur enzymes of *Staphylococcus aureus* – a computational approach

Kannaiah Surendirakumar[1,2] · Wairokpam Sanahal Devi[1] · Subramaniyan Vaithilingam[3]

Received: 24 April 2023 / Revised: 27 July 2023 / Accepted: 12 September 2023

Abstract
Endophyte fungus *Phoma herbarum* (NFCCI 4035) was previously isolated and identified from healthy leaf tissue of *Meriandra bengalensis* Benth plant from Manipur. We recently established the antibacterial activity of ethyl acetate extracts of endophyte fungus *P. herbarum in vitro* and identified some potentially active components using GC-MS. The current study aims to perform molecular docking of the discovered *P. herbarum* compounds against Mur enzymes (Mur A, Mur C, Mur D, and Mur F) of *Staphylococcus aureus* using Auto Dock Tools 1.5.6. SwissADME online tool was used to calculate the drug-likeness characteristics. According to the findings, only 14 of 23 bioactive compounds evaluated from *P. herbarum* extract adhered to Lipinski's Rule of Five (LRo5) and had binding affinity ranged between − 3.5 to -6.5 (kcal/mol) with at least one of the four targeted Mur enzymes. When compared to all other bioactive compounds that interact with target Mur enzymes, 2-Palmitoylglycerol molecule demonstrated highest binding affinity (-6.5 kcal/mol) with Mur F ligase. However, (1R,2R,3R,5 S)-2,6,6-Trimethylbicyclo[3.1.1]heptan-3-amine has shown excellent binding affinity for all selected target (Mur A, Mur C, Mur D, and Mur F) enzymes. Also, this study confirmed that the bioactive compounds can be developed into more potent inhibitors targeting *S. aureus*-related infections.

Keywords Endophytic fungi · Bioactive chemicals · Mur enzymes · Molecular docking · Drug-likeness

Introduction

Endophytes act as biological archives for unique natural chemicals, opening up new avenues for medication development. In the hunt for novel chemical entities, plant-associated microorganisms, including bacteria and fungi that inhabit the internal tissues of all plant species, are becoming more and more important candidates for bioprospecting (Staniek et al. 2008; Tiwari et al. 2021). Endophytic fungus has been linked to the discovery of numerous significant bioactive compounds (Mousa and Raizada 2013). *Penicillium* and other endophytic fungal species have received more attention than other microbial species ever since the discovery of penicillin. They have strong track record of producing a wide range of chemical compounds that fall into several classes, such as alkaloids, antibiotics, hormones, mycotoxins, etc. (Mousa and Raizada 2013; Frisvad et al. 2013). These species are notable for the presence of particular mycotoxins such as patulin, citrinin, ochratoxin, etc., as well as the large number of pharmacologically significant chemicals that have so far been described from them (Tiwari et al. 2021). The rise of resistance to antibiotics by pathogenic species such as *Staphylococcus aureus*, *Streptococcus pneumoniae*, *Pseudomonas aeruginosa*, etc. has become increasingly common and poses a serious threat to public health. In particular, infections related to *Staphylococcus aureus* (*S. aureus*) pathogens have not only become more prevalent but have also started developing resistance

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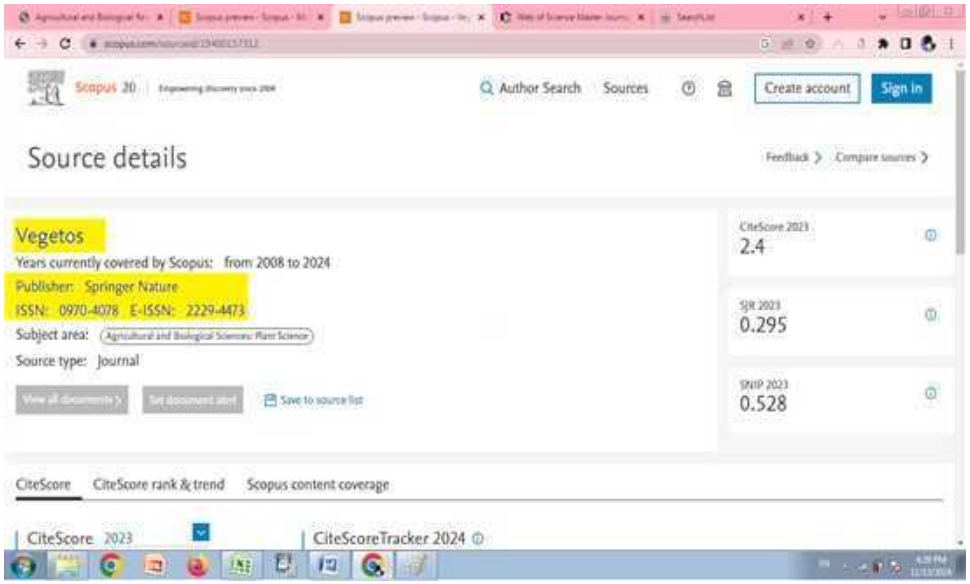

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University of Calcutta, Kolkata 700 019, India

Assessment of root colonization, identification, and phosphate solubilization activity of root endophytic fungi obtained from hybrid tomato *Lycopersicon esculentum* Mill. var. TNAU CO3

KANNAIAH SURENDIRAKUMAR[1,2*], SALINI RAJENDRAN[1], RADHA RAMAN PANDEY[2] , SALAM NIRMALASHACHI CHANU[2], AND PANDIYAN JEEVAN[1]

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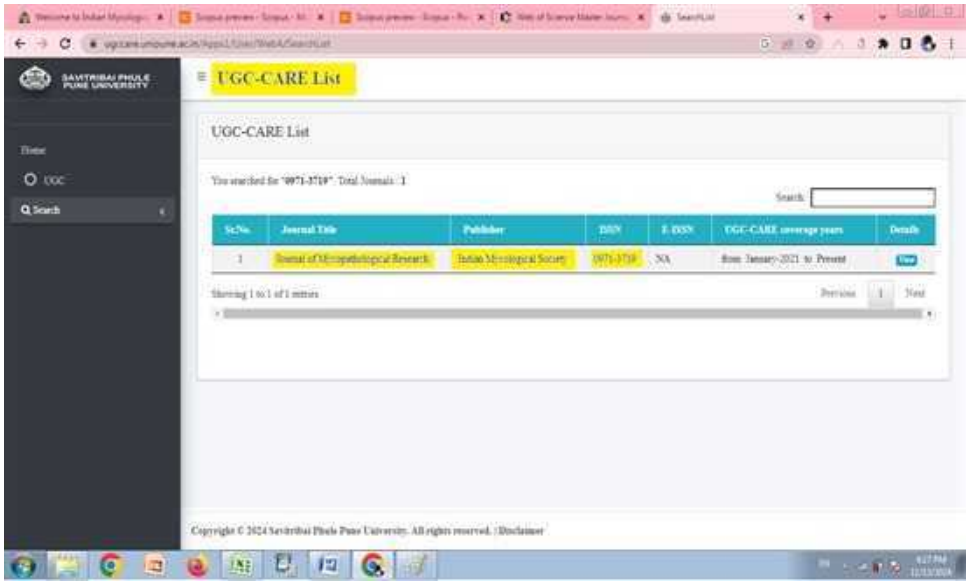
Land plants, in general, rely heavily on positive interactions with fungal endophytes for growth, disease resistance, and stress tolerance. Root colonization, isolation and tri-calcium phosphate (TCP) solubilizing activity of root endophytic fungi (REF) obtained from hybrid tomato (*Lycopersicon esculentum* Mill. var. TNAU CO3) plants grown in natural fields were examined. All field-collected tomato roots were positively colonized by DSE (dark septate endophyte) fungi. A total of 94 culturable fungal isolates belonging to 8 distinct orders, 9 genera, and 11 species were recovered and identified by morphological examination. In *L. esculentum* roots, the endophytic fungal colonization rate (CR%) was noticeably high (62.67%). *Aspergillus niger* was the dominant fungus with a relative abundance (RA%) of 23.4%, while *A. niger*, *Cladosporium cladosporioides*, and *Fusarium oxysporum* had the maximum isolation frequency (IF%). Furthermore, we evaluated the nature of the identified fungal isolates as endophytes by a pot study. Thus, 9 of 11 fungi colonized the test plant roots with clear intracellular structures, including *Alternaria* spp., *C. cladosporioides*, *Colletotrichum* spp., and *F. oxysporum*, which are DSE fungi. Furthermore, four REF were able to solubilize the TCP, with SI% ranging from 1.3 to 2.4%. This study's findings will help to improve our understanding of REF interactions and their potential ability to solubilize inorganic phosphate, as well as the application of these fungi to increase the development and productivity of diverse agricultural plants in sustainable agriculture.

Keywords: Dark septate endophyte fungi, crop plants, colonization, PVK agar, phosphate soubilization



INTRODUCTION

Plant roots are quickly colonized in natural habitats by a vast range of microorganisms, including archaea, bacteria, and endophytic fungus, known as the plant microbiome (Liu *et al.* 2017). Arbuscular mycorrhizal (AM) fungi, the most widespread endophytic fungi in plant roots, form symbioses with about 90% of plant species in all habitats (Smith and Read, 2008).

However, dark septate endophytes (DSE) or root-endophytic fungi (REF) also colonize plant roots alongside AM fungi in tropical, arctic, and alpine habitats (Addy *et al.* 2005; Newsham, 2011). Darkly colored (melanin), septate hyphae, and compact microsclerotial structures define DSE fungi. Plants grown in extreme environments, like heavy metal-polluted soils, low nutrient and high salinity soils, upland agroecosystems, and cold conditions, etc., have high DSE prevalence in their roots. It has also been hypothesized that DSE are mostly non-mycorrhizal plant root-inhabiting fungus.

The majority of previous studies on endophytic fungi have focused on their isolation from aerial plant parts (leaf, stem, flower) and from various crop species such as chilli (*Capsicum annuum*) (Paul *et al.* 2012), potato (*Solanum tuberosum*) (Yasser *et al.* 2019), rice (*Oryza sativa*, *Oryza granulate*) (Naik *et al.* 2009; Yuan *et al.* 2010),

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IN SILICO STUDIES OF *BYTTNERIA HERBACEA* Roxb. BIOACTIVE COMPOUNDS AGAINST ANTI-INFLAMMATORY (COX-1) PROTEIN

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ABSTRACT

The present study explored the potential of *Byttneria herbacea* Roxb. against inflammatory disease by conducting molecular docking studies. The SwissADME tool was utilized to perform a drug-likeness study, which was then followed by molecular docking using the AutoDock 4.2 software. *In silico*, GC-MS research identified 21 molecules, subsequently evaluated for drug-likeness properties. Based on the ADME analysis, six compounds were recognized as superior compounds. The docking analysis of these six molecules was performed with Autodock 4.2. Finally, two compounds were shown to be effective against Cyclooxygenase-2: 7-Methoxy-2,2-dimethyl-2H-1-benzothiopyran and 3-buten-2-one, 4-(5,5-dimethyl-1-oxaspiro[2.5]oct-4-yl) against the enzyme (COX-1). Excellent docking properties and the lowest binding energy (-6.94 and -6.90 kcal/mol) were also found. According to the data, *B. herbacea* aerial plant component showed a significant anti-inflammatory molecular docking effect.

Keywords: Anti-inflammatory activity; AutoDock; *Byttneria herbacea*; Molecular docking; Drug likeness

INTRODUCTION

Byttneria herbacea Roxb. (Family: Malvaceae) is a plant that is often found in peninsular India (Gujarat, Tamil Nadu, Odisha, and Bihar) and is known as a favorite odder (Khas) of deer (Sambar/Samar). Previous research has shown that indigenous societies employ the *B. herbacea* crude medication as a treatment for a variety of illnesses (**Sharma and Acharya, 2018**). It is effective in relieving bodily discomfort when taken orally (**Sreeramulu *et al.*, 2012; Maith *et al.*, 2010; Sathish *et al.*, 2021**). Diarrhea and gynecological issues are treated with the whole plant. The Odisha people have used the roots and leaves as vegetables (**Sharma *et al.*, 2020**). In our earlier study, we reported the whole plant phytochemical profile of methanol extract bioactive compounds from *B. herbacea* plant and analyzed by GC-MS and revealed 24 compounds (**Sathish *et al.*, 2021**). In addition, other researched also showed a significant antioxidant, antimicrobial activity (**Sharma and Acharya, 2018, 2020**). But very few studies are reported on *in silico* approaches.

Infection and injuries cause inflammation. It is linked to arthritis, cancer, stroke, and other neurological and cardiovascular diseases (**Nathan, 2002**). Due to their enhanced biological synthesis in inflamed tissue, prostaglandins (PGs) are the key competitors in forming the inflammatory response (**Stables, 2011**). COXs (prostaglandin G/H synthases) are bifunctional enzymes that act as COX and a peroxidase. They exist in two different isoforms i.e. COX-1 and COX-2, and both are required for prostaglandin G/H synthesis (**Smith, 2000**). Despite their essential similarity, their expression profiles are substantially different. COX-2 is generally referred to as a "housekeeping enzyme" in the medical profession because it is primarily involved in physiological tasks such as maintaining and safeguarding renal function and controlling platelet aggregation via activation of the enzyme thromboxane A2 (TXA2). On the other hand, COX-1 is thought to be primarily essential for initiating and maintaining the inflammatory response, with minor physiological effects such as boosting prostacyclin (PGI2) production and decreasing platelet aggregation (**Oniga, 2017**).

In silico protein analysis is a legitimate alternative research method at the molecular level. In drug design and discovery, molecular modeling and docking are most frequently used in this context. The molecular docking approach aids in the determination of the optimal binding orientation of single or multiple drugs to their target proteins, which are responsible for the development of illnesses and diseases. Sampling and scoring are two of the essential features of protein-ligand docking software. When a protein's binding site is sampled, it generates a variety of ligand-binding conformations. Scoring predicts the tightness of binding for various ligand conformations using a physical or empirical energy function (**Shoichet *et al.*, 2002**).

The binding mode is expected to be the top conformation. The three fundamental components of protein-ligand docking are system representation, conformational space search, and rating of candidate solutions. In docking, the scoring functions are solely responsible for the binding energy of the target proteins and the ligand. The docking score is derived based on the free energy required for binding (**Holt *et al.*, 2008**).

MATERIAL AND METHODS

Target Protein Selection

The docking analysis focused on the anti-inflammatory COX-1 protein (PDB ID: 6Y3C). The docking configurations were collected from the PDB (https://www.rcsb.org/structure/6Y3C). COX-1 binding sites were ligand-free (Fig. 1). Protein heteroatoms were eliminated and replaced by polar hydrogen atoms. Additionally, the proteins were given partial atomic charges. The proteins were allocated molecular solvation parameters, and the data were converted to PDBQT format.

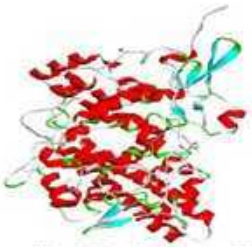

Figure 1 3D Structure of Human COX-1 Crystal Structure (PDB ID: 6Y3C)

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IN SILICO STUDIES OF *BYTTNERIA HERBACEA* Roxb. BIOACTIVE COMPOUNDS AGAINST ANTI-INFLAMMATORY (COX-1) PROTEIN

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Keywords: Anti-inflammatory activity; AutoDock; *Byttneria herbacea*; Molecular docking; Drug likeness

INTRODUCTION

Byttneria herbacea Roxb. (Family: Malvaceae) is a plant that is often found in peninsular India (Gujarat, Tamil Nadu, Odisha, and Bihar) and is known as a favorite odder (Khai) of deer (Sambar Samar). Previous research has shown that indigenous societies employ the *B. herbacea* crude medication as a treatment for a variety of illnesses (**Sharma and Acharya, 2018**). It is effective in relieving bodily discomfort when taken orally (**Sreeramulu *et al.*, 2012**; **Mairh *et al.*, 2010**; **Sathish *et al.*, 2021**). Diarrhea and gynecological issues are treated with the whole plant. The Odisha people have used the roots and leaves as vegetables (**Sharma *et al.*, 2020**). In our earlier study, we reported the whole plant phytochemical profile of methanol extract bioactive compounds from *B. herbacea* plant and analyzed by GC-MS and revealed 24 compounds (**Sathish *et al.*, 2021**). In addition, other researched also showed a significant antioxidant, antimicrobial activity (**Sharma and Acharya, 2018, 2020**). But very few studies are reported on *in silico* approaches.

Infection and injuries cause inflammation. It is linked to arthritis, cancer, stroke, and other neurological and cardiovascular diseases (**Nathan, 2002**). Due to their enhanced biological synthesis in inflamed tissue, prostaglandins (PGs) are the key competitors in forming the inflammatory response (**Stables, 2011**). COXs (prostaglandin G/H syntheses) are bifunctional enzymes that act as COX and a peroxidase. They exist in two different isoforms i.e. COX-1 and COX-2, and both are required for prostaglandin G/H synthesis (**Smith, 2000**). Despite their essential similarity, their expression profiles are substantially different. COX-2 is generally referred to as a "housekeeping enzyme" in the medical profession because it is primarily involved in physiological tasks such as maintaining and safeguarding renal function and controlling platelet aggregation via activation of the enzyme thromboxane A2 (TXA2). On the other hand, COX-1 is thought to be primarily essential for initiating and maintaining the inflammatory response, with minor physiological effects such as boosting prostacyclin (PGI2) production and decreasing platelet aggregation (**Oniga, 2017**).

In silico protein analysis is a legitimate alternative research method at the molecular level. In drug design and discovery, molecular modeling and docking are most frequently used in this context. The molecular docking approach aids in the determination of the optimal binding orientation of single or multiple drugs to their target proteins, which are responsible for the development of illnesses and diseases. Sampling and scoring are two of the essential features of protein-ligand docking software. When a protein's binding site is sampled, it generates a variety of ligand-binding conformations. Scoring predicts the tightness of binding for various ligand conformations using a physical or empirical energy function (**Shoichet *et al.*, 2002**).

The binding mode is expected to be the top conformation. The three fundamental components of protein-ligand docking are system representation, conformational space search, and rating of candidate solutions. In docking, the scoring functions are solely responsible for the binding energy of the target proteins and the ligand. The docking score is derived based on the free energy required for binding (**Holt *et al.*, 2008**).

MATERIAL AND METHODS

Target Protein Selection

The docking analysis focused on the anti-inflammatory COX-1 protein (PDB ID: 6Y3C). The docking configurations were collected from the PDB (https://www.rcsb.org/structure/6Y3C). COX-1 binding sites were ligand-free (Fig. 1). Protein heteroatoms were eliminated and replaced by polar hydrogen atoms. Additionally, the proteins were given partial atomic charges. The proteins were allocated molecular solvation parameters, and the data were converted to PDBQT format.

Figure 1 3D Structure of Human COX-1 Crystal Structure (PDB ID: 6Y3C)